Basics of scattering:

In the Born approximation (that is in systems where the scattering cross-section is small and effects such as attenuation with thickness and multiple scattering do not need to be considered) we can describe the neutron or x-ray scattering process for any arbitrary system by

$$A_{discreet} \prec \sum_{j\_scatterers} b_{c_j} e^{iQ\cdot R_j} = \sum_{j\_scatterers} b_{c_j} \left\{\cos(Q\cdot R_j) + i\sin(Q\cdot R_j)\right\}$$

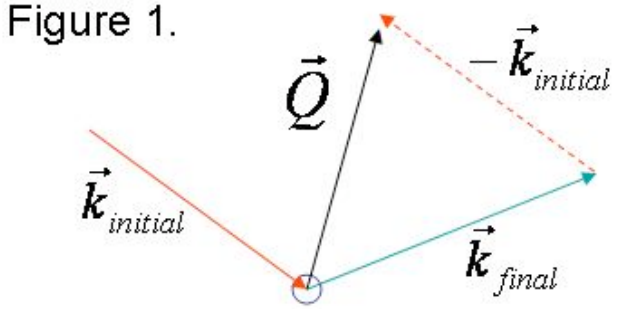
$$A_{continuous} \prec \int_{volume} \rho b_c e^{iQ\cdot R} dv = \int_{volume} \rho b_c \left\{\cos(Q\cdot R) + i\sin(Q\cdot R)\right\} dv$$

$$\rho b_c = scattering\_length\_density = SLD$$

$$I(Q) \cong \frac{I_O}{Area} |A|^2 \frac{\Delta\Omega}{4\pi^2}$$

A is the scattering amplitude (just like the amplitude of any wave), and bc is the coherent scattering length density which tells us how strongly the material scatters. For neutrons bc is given in units of Å-2 (typically on the order of 1-10 x 10^-6 Å2), while for x-rays it is given by f and f'(in units of the electron radius, ro = 2.52 x 10-5 Å) times the material density in Å-3, the latter being imaginary (i.e. absorbing). bc can also have an imaginary component, but for the neutrons energies we will be working with it this imaginary term is negligible. Q is the scattering wave vector whose direction is determined by the subtraction of the incoming wave direction from the scattered wave (Figure 1), and whose magnitude is $2\pi/\lambda$ with λ = wavelength. (We will discuss where the more about Q shortly.) Rj is the relative position in space of the jth scatterer with respect to all the other scattering centers. We don't need to know the actual location in space of R relative to the incoming wavefront since we loose this phase information when we square A to get the measured intensity, I. Finally, you will notice that an exponent of an imaginary number can be written in wave-compatible terms of sines and cosines.

Figure 1.



$$\vec{Q} = \vec{k}_{final} - \vec{k}_{initial}$$

$$\left|\vec{k}_{initial}\right| = \left|\vec{k}_{final}\right| = \frac{2\pi}{\lambda}$$

To understand how these equations work, especially Q, let's examine two common scattering geometries. It is often easiest to think of scattering in terms of constructive and destructive interference between two waves depending on their relative phases (i.e. if the

phase difference is zero or any integer multiple of 2π then their amplitudes add and I_total = 4I_single, but if the phase difference is multiples of π apart then the waves are out of phase and we record zero intensity). In truth if is actually the neutron (or x-ray) wave-function that interferes with itself (as in the 2-slit experiment) that gives rise to the observed pattern, but the mathematics is the same so it's easier to picture the situation as arising from the interference of classical, discreet waves.

I. Transmission through a thin slab

The path length difference is $\Delta = d\sin(\theta)$, which at maximum constructive interference $= n\lambda$, can be rewritten as $\frac{2\pi\sin(\theta)}{\lambda} = \frac{2\pi}{d}$. Under this condition $\sin(\theta) = 1$ so $|Q| = \frac{2\pi}{\lambda} \Rightarrow \frac{2\pi}{d}$. For this reason when we see a prominent scattered peak we typically say it originates from a structure with a periodic spacing of d, or a Q of $\frac{2\pi}{d}$.

Now let's approach this same situation using the conventional reciprocal space notation – that is in terms of Q from the start. Using vector notation,

$$\vec{Q} = \frac{2\pi}{\lambda}\left[\cos(\theta) - 1, \sin(\theta), 0\right]$$

Since we care only about the relative positions our scatterers let's write define one of the scatterers to be located at the origin:

$$\vec{R}_1 = (0,0,0)$$
$$\vec{R}_2 = (0,d,0)$$

Now $I = \left|e^{i(0)} + e^{i(\frac{2\pi}{\lambda}\sin(\theta)d)}\right|^2 = \left|1 + \cos(\frac{2\pi}{\lambda}\sin(\theta)d)\right|^2 + \left|\sin(\frac{2\pi}{\lambda}\sin(\theta)d)\right|^2$. This is maximized when $\frac{\sin(\theta)}{\lambda} = \frac{1}{d}$, the same conclusion we reached using basic geometry. A plot of this 2-particle scattering as a function of Qy is shown in Figure 3.

The beauty of using reciprocal space (Q-notation) is that can be used easily for much more complicated 3-D scattering distributions and for multiple particles all scattering and interfering with one another simultaneously. Try adding a third particle at (0,2d) or even one at an arbitrary (x,y) and you'll see how much easier working in reciprocal space becomes!

II. Specular reflectivity

Reflectivity in general means reflecting off of a smooth surface, such as off your typical silver-coated mirror. Specular reflectivity is a special case where the incident and scattered angles are the same, Figure 4.

Here I have rotated the axes since the reflectivity community typically uses z to denote the direction perpendicular to the sample plane. From geometry you can deduce that $\Delta = 2d\sin(\theta)$ in which maximum scattering occurs at $\frac{2\sin(\theta)}{\lambda} = \frac{1}{d}$. In the Figure you can see that $\vec{Q} = \frac{2\pi}{\lambda}(0,0,2*\sin(\theta))$ or $Q_Z = \frac{4\pi\sin(\theta)}{\lambda}$. Since we can only observe the component of the difference in scattering position for which there is a non-zero Q-component, a key feature of specular reflectivity is that in this geometry we are only sensitive to the depth-dependence, but not any in-plane structures. Using reciprocal space we can calculate the scattering from two particles as

$\vec{R}_1 = (0,0,0)$

$\vec{R}_2 = (x,y,d)$

Where $I = \left|e^{i(0)} + e^{i(\frac{4\pi}{\lambda}\sin(\theta)d)}\right|^2 = \left|1+\cos(\frac{4\pi}{\lambda}\sin(\theta)d)\right|^2 + \left|\sin(\frac{4\pi}{\lambda}\sin(\theta)d)\right|^2$, and we see a maxima at $\frac{2\sin(\theta)}{\lambda} = \frac{1}{d}$ (again same result as from basic geometry). The scattering from this system is given in Figure 5, and doubles in frequency from the transmission case for the same spacing, d. Scattering for a crystal of .. Figure 6. (In reality for real samples with many scattering centers when you go to very low angles (very small Q) the Born approximation no longer holds and multiple scattering must be accounted for, but we will deal with this in the next section.)

III. Off-specular (or diffuse) reflectivity

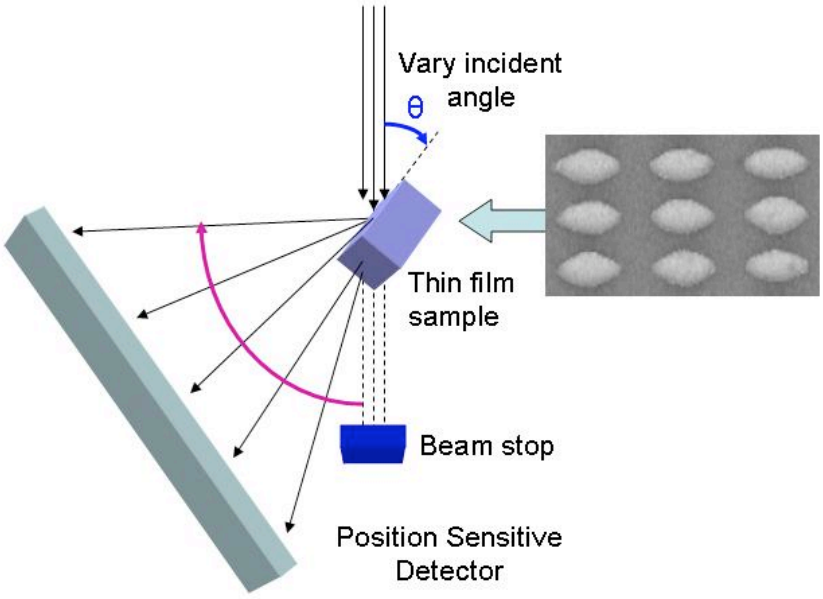
Your research project does not go into this, but you will be involved in taking data for such a system (nanoparticles monolayer) so you might as well see what it is. Sometimes you …

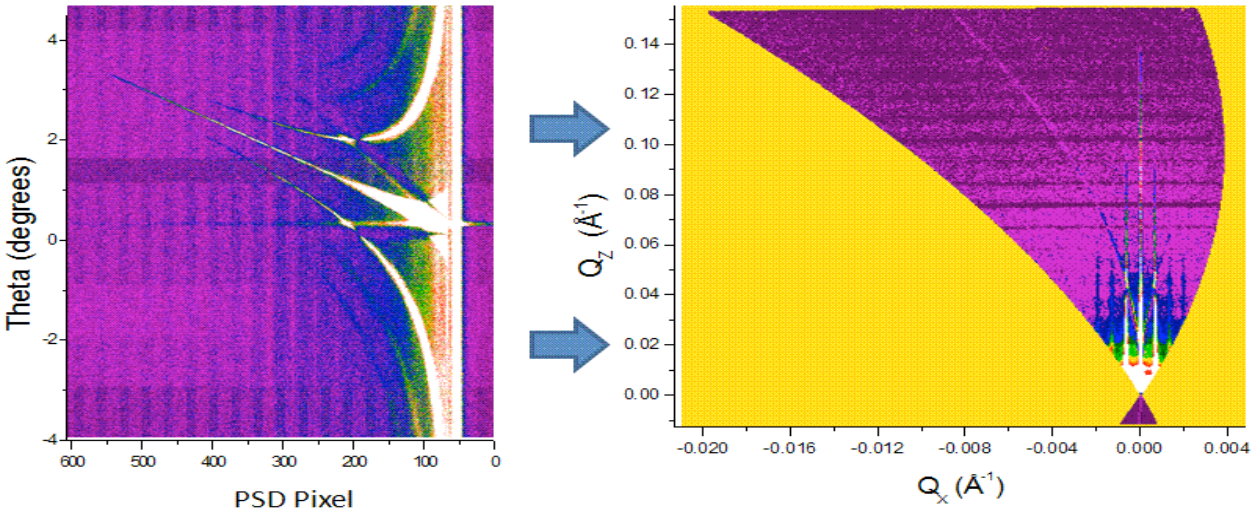
$$Q_X = \frac{2\pi}{\lambda}\{\cos(\theta_f - \theta_i) - \cos(\theta_i)\}$$

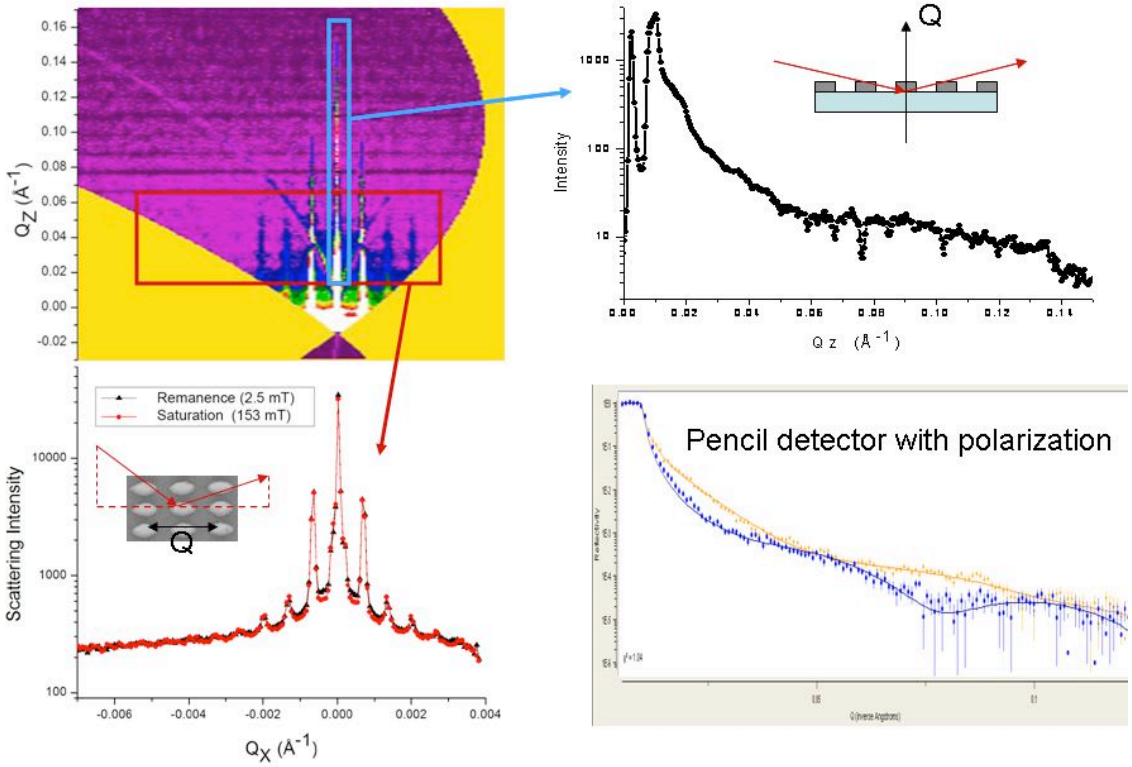
$$Q_Z = \frac{2\pi}{\lambda}\{\sin(\theta_f - \theta_i) - \sin(\theta_i)\}$$

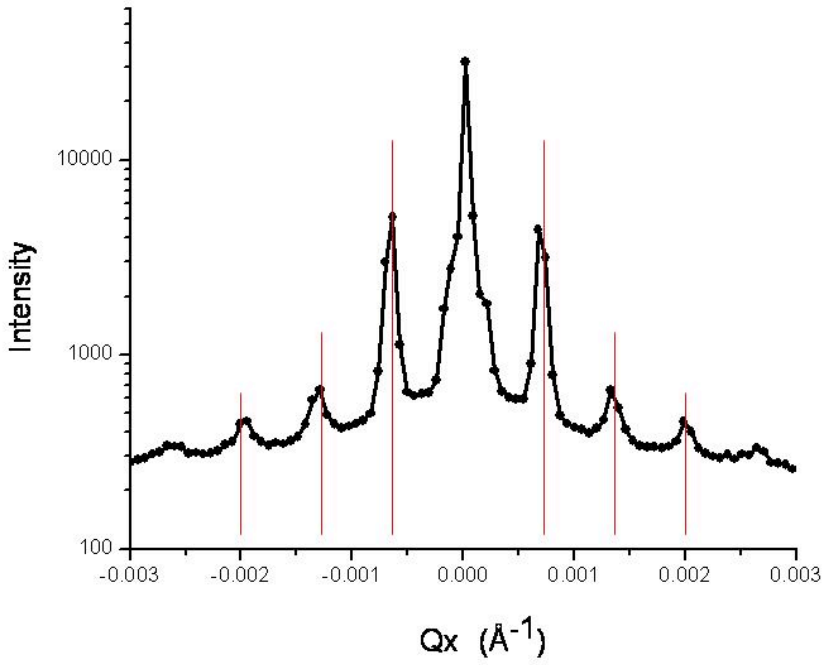
For off-specular: $Q_X = \frac{2\pi}{\lambda}\left(\sin(\theta_{final}) + \sin(\theta_{initial})\right), Q_Z = \frac{2\pi}{\lambda}\left(\cos(\theta_{final}) - \cos(\theta_{initial})\right), Q_Y$ is not considered since we have no detector resolution in this direction. You will note that

it is much easier to reach high values of Qx than Qz. Figure 7 shows a representative data set for patterned ellipses with a periodic spacing of 9000 Å.









Peaks are at:

0.000 Å-1

± 0.007 Å-1

± 0.014 Å-1

± 0.021 Å-1

Q = 2π / D

Thus, widths are:

9000 Å (D / 1.0)

4500 Å (D / 2.0)

3000 Å (D / 3.0)